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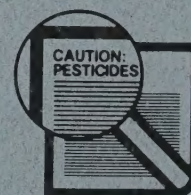# AN EXAMINATION OF THE NONWATER EVAPORATION ALGORITHM IN FSCBG

An Examination of the
Nonwater Evaporation Algorithm
in FSCBG

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# SUMMARY

The nonwater evaporation algorithm in FSCBG (Forest Service Cramer-Barry-Grim) is examined in detail. Its equation foundation, sensitivity of model inputs, and validation with water-based spray materials are discussed. The use of an auxiliary computer program to develop the inputs needed for the nonwater algorithm is explained, including a user manual for the operation of the program. A review of previous nonwater-based experimental measurements is made, and their relationship with each other, and the simple evaporation laws commonly assumed, are presented.

Overall, the continued use of the water-based evaporation formula in FSCBG is warranted, even with nonwater-based spray materials. However, care must be taken to ensure that the proper nonvolatile fraction for this material is input into FSCBG.

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# 1. INTRODUCTION

The development of the aerial application model FSCBG (Forest Service Cramer-Barry-Grim) has spanned more than fifteen years, from the release of its first version (Dumbauld, Bjorklund and Saterlie 1980), to a second version containing the near-wake AGDISP model (Bjorklund, Bowman and Dodd 1988), on to the release of the 4.0 version containing a completely rewritten user interface and scientific code (Teske and Curbishley 1991; Teske, Curbishley and Skyler 1991; and Teske et al. 1993). The latest upgrade to the model is its 4.3 version (Teske and Curbishley 1994).

One of the linchpins in FSCBG is its evaporation module, whose development draws heavily upon accepted engineering approximations, including Fuchs (1959), Beard and Pruppacher (1971), Goering, Bode and Gebhardt (1972) and Williamson and Threadgill (1974). Its fundamental equation expresses the time rate of change of drop diameter due to evaporation (Teske et al. 1993) as

$$\frac{dD^2}{dt} = -\frac{4\,M_V\,D_V\,\rho_A\,(e_S - e_\infty)}{M_m\,\rho_V\,(P_A - e_S)}\,Sh \qquad (1)$$

where

$M_V$ = molecular weight of evaporating vapor from the drop (gm per mole)

$M_m$ = mean molecular weight of the resulting vapor-air mixture, approximated by air $M_A$ (gm per mole)

$D_V$ = molecular diffusivity of the evaporating vapor in air at the drop temperature (sq cm per sec)

$D$ = drop diameter (cm in this equation)

$\rho_A$ = air density (gm per cu cm)

$\rho_V$ = drop density (gm per cu cm)

$e_S$ = partial pressure of the evaporating vapor at the drop surface (mb)

$e_\infty$ = partial pressure of the evaporating vapor far from the drop (mb)

$P_A$ = ambient air pressure (mb)

$Sh$ = Sherwood number

$t$ = time (sec)

This particular equation solves for the evaporation of water-based droplets, although FSCBG (in its "Advanced" user level) includes a nonwater evaporation algorithm. To our knowledge, the nonwater evaporation algorithm has not been explored in any detail previously, although its presence in FSCBG indicates that the original architects of the code intended a place for it. Thus, it seems fitting to examine this particular algorithm in FSCBG, specifically to see whether it may be useful in those applications where the tank mix is nonwater-based. This investigation is the focus of the present report.

This report will first review the nonwater algorithm in FSCBG, then move to an examination of the physical properties that must be entered into the code to enable it to solve a nonwater tank mix evaporation problem. An extended discussion of a separate program (called NONWATER) then occupies a portion of this report (including an Appendix that contains its user manual). Following is then an examination of experimental evaporation data, including a look at a simple approach to evaporation. Lastly, recommendations are offered on the use of the nonwater options in FSCBG.

# 2. FSCBG NONWATER ALGORITHM

With the selection of "nonwater" Carrier Type in FSCBG (in its "Advanced" user level), and selecting Physical Constants from the Spray Material menu, the following rather forbidding menu appears:

```
BGI Data>Spray Mat>Phys Cons

        Physical Constants

        A-Molecular Weight                     18.01 g/mol
        B-Diffusivity                          none  cm2/s
        C-Latent Heat of Vaporization          none  cal/g
        D-Molal Concentration                  none  mol/cm3
        E-Ambient Vapor Pressure               none  mb
        F-Thermal Conductivity                 none  cal/deg k_cm_s
        G-Vapor Pressure Coefficient B          3.00 ln mb
        H-Vapor Pressure Coefficient C        258.55 (ln mb)_deg k
```

with the default values as shown. This menu defines the variables that must be entered by the user for evaporation of nonwater-based spray materials. Within the applications discussed here, these variables may be defined as follows:

1. Molecular Weight $M_v$. The weight of a molecule of the tank mix (the default is the molecular weight of water, containing two Hydrogen atoms -- with a weight of approximately 1 gm per mole -- and one Oxygen atom -- with a weight of approximately 16 gm per mole; the exact weight is just slightly over this sum).

2. Diffusivity $D_v$. The net transport of a molecule through the air, denoted by the rate of diffusion of the evaporating vapor into the air, due to intermolecular collisions rather than turbulence or bulk fluid transport. A typical value for the diffusion coefficient of water through air is 0.234 sq cm per sec.

3. Latent Heat of Vaporization L. The quantity of heat required to convert a unit mass of liquid into a vapor without raising its temperature (through a constant pressure process). The latent heat of vaporization of water at 20 deg C is 590.6 cal per gm.

4. Molal Concentration $C_f$. The concentration of the air-liquid mixture. A typical value for the molal concentration of water in air is 0.00004134 moles per cu cm, which is in fact the ratio of air density (0.001197 gm per cu cm) divided by the molecular weight of air (28.97 gm per mole).

5. Ambient Vapor Pressure $e_\infty$. The partial pressure of an evaporating material in the local environment. For water vapor the ambient pressure (in mb) may be determined from the expression (Rasmussen 1978)

$$e_\infty = \beta \left[ \frac{575.0466 + 31.82291\, T_A + 1.296028\, T_A^2}{93.51611 - T_A} \right] \tag{2}$$

where $\beta$ is replaced by the relative humidity expressed in fractional form and $T_A$ is the ambient temperature in deg C. This expression recovers an ambient vapor pressure of 14.12 mb at a temperature of 20 deg C and a relative humidity of 60 percent. For evaporating materials not usually found in the atmosphere, an ambient vapor pressure of zero is recommended (Dumbauld, Bjorklund and Saterlie 1980).

6. Thermal Conductivity k. The quantity of heat which will traverse a medium of unit thickness and cross-sectional area per unit time, under the influence of an applied temperature gradient. In the case of evaporation the relevant thermal conductivity is of the air-gas mixture surrounding the drop at the drop surface temperature. A typical value for the thermal conductivity of vapor surrounding a water drop is 0.00005905 cal per deg K per cm per sec.

7. Vapor Pressure Coefficients B and C. The vapor pressure at the surface of the drop, expressed by a two-parameter relationship, sometimes called the Clapeyron equation (Reid, Prausnitz and Poling 1987)

$$p_{vb} = \exp [\, B - C / T \,] \tag{3}$$

where $p_{vb}$ is the vapor pressure in mb and T is temperature in deg K. For the ambient temperature and relative humidity cited above, a water drop would exhibit water vapor with a partial pressure of 17.02 mb and temperature of 14.92 deg C. A consistent vapor pressure may be found from Eq 3 with B $= 3.0$ (ln mb) and C $= 47.7$ (ln mb) deg K.

In the evaporation process the critical relationship is that of a compatible drop temperature with drop pressure. An expression for the drop temperature $T_d$ (in deg C) of a nonwater drop may be found by applying the principle of conservation of energy at the drop surface. Balancing the loss of latent heat with the gain of heat by conduction, an expression for the temperature difference between ambient and drop surface may be developed (Beard and Pruppacher 1971) to give

$$T_A - T_d = \frac{C_f \, D_v \, L}{k \, M_v} \frac{(p_{vb} - e_\infty)}{(P_A - p_{vb})} \frac{Sh}{Nu} \tag{4}$$

where

$$Nu \quad = \quad \text{Nusselt number}$$

Simplifying Eq 4 by dropping the Sh / Nu term, and substituting for $p_{vb}$ from Eq 3 gives

$$T_d = T_A - \frac{C_f \, D_v \, L}{k \, M_v} \frac{[\exp (B - C / T_d) - e_\infty]}{[P_A - \exp (B - C / T_d)]} \tag{5}$$

resulting in a nonlinear equation for the drop temperature $T_d$. In FSCBG this equation is solved by a Newton-Raphson iteration to recover the drop temperature and, with the use of

Eq 3, drop pressure. This solution procedure is consistent with the approach used in the U. S. Army DROP code (Sommerville 1992) adapted from several subroutines of the larger NUSSE4 model (Pennsyle 1992).

# 3. SENSITIVITY STUDY

One of the first steps toward understanding the nonwater algorithm in FSCBG is to understand the relative importance of the various inputs into Eq 5 above. Thus, our next step is an examination of the sensitivity of evaporation to the physical properties of the nonwater spray material.

Our approach is the following: a single droplet size (200 micrometers in diameter) is examined in detail. First, the water-based evaporation is developed, then the nonwater evaporation representing the same physical parameters is recovered, then a sensitivity study is performed around these parameters with the nonwater evaporation algorithm. Because of the way in which the evaporation results are used in the code (for later dispersion calculations which are not important here), a quadratic curve fit is always performed by FSCBG to recover the evaporation effect by the expression

$$D = a + b\,t + c\,t^2 \tag{6}$$

where (a,b,c) are constants developed from the evaporation results by a least-squares technique. Since in our sensitivity study the first constant a (in Eq 6) will always be the initial droplet size of 200 micrometers, we examine the next most important constant b by comparing its sensitivity to various physical property changes. We follow a comparison procedure similar to that employed in Teske and Barry (1993) by computing

$$\text{Sensitivity Factor} = \frac{(B_v / B_{base}) - 1}{(V_v / V_{base}) - 1} \tag{7}$$

where $V_v$ and $B_v$ are the assumed variable value and its resulting b coefficient value, respectively, and $V_{base}$ and $B_{base}$ are the base value and b coefficient around which the sensitivity is performed, respectively. Thus, it may be seen from Eq 7 that if the variable is doubled in value, resulting in a b coefficient that also doubles, the resulting sensitivity factor is 1.0 -- there is a one-for-one change in evaporation characteristics with the physical property examined. Clearly, the larger the sensitivity factor the more sensitive the variable. The sensitivity results are summarized in Table 1. Note that the base temperature and relative humidity are 20 deg C and 60 percent, respectively.

Several observations may be made from this study:

1. The vapor pressure coefficients B and C are both critical inputs to the nonwater evaporation algorithm, with B especially sensitive. Thus, this study would suggest that the use of the nonwater algorithm requires a correct and accurate description of the vapor pressure effect in the nonwater spray material before running FSCBG. Otherwise, because of the level of sensitivity to the B coefficient, the results from FSCBG will be speculative at best. Resource books on physical properties generalize Eq 3 into a form first suggested by Antoine (1888)

$$p_{vb} = \exp\,[\,B - C\,/\,(T + A)\,] \tag{8}$$

where the additional constant A has been added to the description for $p_{vb}$, extending the accuracy of the expression but adding further complication. Although estimation techniques are available to recover the vapor pressure coefficients (as discussed in the next section of this report), these rules may be considered occasionally unreliable, and the only accurate way to obtain values of these constants is to correlate experimental results (Reid, Prausnitz and Poling 1987).

2. The ambient vapor pressure is seen to be quite important here (a negative sign in the last column in Table 1 indicates that an increase in the parameter results in a decrease in the constant b and, therefore, a decrease in the evaporation rate). It is in fact the difference between the vapor pressure at the drop and the ambient vapor pressure that drives Eq 5 to a solution for drop temperature (in other words, when the vapor pressure gradient goes to zero at the surface of the drop, evaporation ceases). For spray materials not present in the atmosphere, an ambient vapor pressure of zero must be assumed, and the sensitivity of this variable is irrelevant. On the other hand, if the nonwater spray material is mixed with water, the ambient vapor pressure of water may be assumed here. Since this pressure is computed by the evaporation algorithm, the sensitivity of this variable is again irrelevant.

3. Eq 1 shows that droplet evaporation is directly proportional to the molecular weight; thus, it is not surprising that the sensitivity to molecular weight is nearly one-to-one. Again, the molecular weight of the nonwater material must be known accurately (in the case of a tank mix, the mass-averaged molecular weight should be used).

4. Eq 1 also shows that droplet evaporation is directly proportional to the diffusivity; in addition, the Sherwood number may be defined (Pruppacher and Rasmussen 1979) as

$$Sh = 1.56 + 0.616 \, Sc^{1/3} \, Re^{1/2} \qquad Sc^{1/3} \, Re^{1/2} > 1.4 \qquad (9)$$

with appropriate correction to $Sh = 2.0$ as $Sc^{1/3} \, Re^{1/2}$ approaches zero (Froessling 1938 and Wedding, Kim and Dennison 1986). Here Sc is the Schmidt number, defined by

$$Sc = \frac{\mu_A}{D_v \, \rho_A} \qquad (10)$$

and Re is the Reynolds number

$$Re = \frac{V \, D \, \rho_A}{\mu_A} \qquad (11)$$

where

$\mu_A$    =    absolute viscosity of air (gm per cm per sec)

$V$    =    drop velocity (cm per sec)

Thus, the presence of diffusivity in the Schmidt number modifies the sensitivity of evaporation rate slightly.

5. The other three variables examined here (latent heat of vaporization, molal concentration, and thermal conductivity) are relatively unimportant in the evaporation process, and may be taken at their water-based values. This result is a significant finding of the sensitivity study, because it means that we do not have to seek expressions for these three variables, but can always implement the water values computed in FSCBG. This finding is especially important for thermal conductivity, because its accurate analytical expression is extremely complicated (Lyman, Reehl and Rosenblatt 1990).

6. Temperature does not seem to have a strong effect on sensitivity, for variations around the selected default value of 20 deg C, whereas relative humidity does. It should not be implied from this conclusion, however, that nonwater evaporation is insensitive to temperature in all applications. A quick look at Table 1 shows that the variation of temperature is nearly as important as diffusivity.

Our purpose here is to seek an analytical technique to recover estimates of the more important variables in the nonwater evaporation algorithm. Clearly, the best way of dealing with these variables is by laboratory experiments constructed to recover these parameters precisely, although this approach is impractical for all tank mixes considered by the USDA Forest Service. Thus, an alternate approach is desired, and one such technique is a property estimation program refined by the U. S. Army. This estimation approach is covered in the next section of this report.

Table 1: A Sensitivity Study of the Nonwater Inputs to FSCBG

| Variable | Base Value | Sensitivity Factor |
|---|---|---|
| Vapor Pressure Coefficient B | 3.0 (ln mb) | 18.338 * |
| Ambient Vapor Pressure | 14.12 mb | -4.656 |
| Molecular Weight | 18.01 g/mol | 0.943 |
| Vapor Pressure Coefficient C | 47.7 (ln mb) deg K | -0.902 |
| Diffusivity | 0.234 cm$^2$/sec | 0.769 |
| Latent Heat of Vaporization | 590.6 cal/gm | -0.011 |
| Molal Concentration | 0.00004134 mol/cm$^3$ | -0.011 |
| Thermal Conductivity | 0.00005905 cal/deg K cm sec | 0.011 |
| Temperature | 20 deg C | 0.488 |
| Relative Humidity | 60 percent | -1.380 |

\* An increase/decrease in Vapor Pressure Coefficient B results in more than an 18-fold increase/decrease in the linear evaporation rate term (coefficient b in Eq 6) over the base results. Thus, if B is doubled in the nonwater evaporation algorithm in FSCBG, the evaporation rate will increase by a factor of 2 times 18.338, or 36.676.

# 4. PARAMETER ESTIMATION PROGRAM

The driving force behind the examination of the nonwater algorithm in FSCBG was the acquisition of a property estimation program (appropriately entitled PROPEST, for PROPerty ESTimation) from Aberdeen Proving Ground (Famini 1987). It was thought that this code, which has at times been considered proprietary by the U. S. Army, could be of help in developing the needed parameters for FSCBG implementation of nonwater spray materials. Although we initially thought all of the inputs in the Physical Constants menu would need to be estimated, the above sensitivity study clearly shows that the parameters of interest are: Molecular Weight, Diffusivity, and the Vapor Pressure Coefficients. It is assumed here that the Ambient Vapor Pressure is zero for completely nonwater carriers, and water-like for water-based tank mixes.

Unfortunately, it did not take long to discover that the estimation of physical properties is an inexact science (at best), and requires an intimate knowledge of the molecular structure of the evaporating material. This realization poses a significant problem because we know that biological materials are not easily amenable to molecular analysis. Nevertheless, it seems to make sense to try to apply the program here, in the hopes that some useful information might be extracted from it. This information would (hopefully) serve to provide a scoping, or approximate, look at the spray material in question. Because many materials are in fact mixtures, the program must be run individually for each substance, and a mass-average analysis run to combine the tank mix. It is important, of course, to have some sense of which tank mix materials will evaporate FIRST, since these should be the Vapor Pressure Coefficients used in FSCBG. Herein lies the utility of the program: if the spray material is mixed with water, the material evaporation properties should be checked to see that water will EVAPORATE FIRST. Then, in the FSCBG simulation, the water properties (developed internally by the model) can be used, and the Physical Constants menu does NOT have to be entered or its inputs modified. If, however, a specific spray material clearly will evaporate BEFORE the water base (or at the same time as the water base), then the appropriate tank mixture inputs must be entered into FSCBG. Under most circumstances, with spray materials tested by the Spray Drift Task Force (Teske 1994), the tank mix behaves like water.

This approach does not make light of the difficulty of evaluating the evaporation of a complex solution. When a tank mix is composed of several evaporating components, the need to calculate vapor pressure becomes a significant deterrent to the solution, although detailed approaches (such as Prausnitz, Orye and O'Connell 1967; Picot, Chitrangad and Henderson 1981; and more recently Riley et al. 1994) and laboratory experiments (discussed later) have proven successful.

The Appendix contains a user manual describing the operation of the stand-alone property estimation program NONWATER. The methods implemented for estimating the needed properties were chosen from among the many available techniques in order to obtain accurate results without overly burdensome input requirements. These techniques were extracted from the two main sources Lyman, Reehl and Rosenblatt (1990) and Reid, Prausnitz and Poling (1987), although for each technique used, its specific references will be cited where possible. The program Main Menu appears as shown in Table 2. The entries are as follows:

1. The *molecular weight* is the most straightforward. NONWATER contains all of the elements in the periodic table, with their individual molecular weights, and the user merely constructs the compound to be examined. This requirement, however, may be a

very difficult one to accomplish with some materials, as many biological spray materials may not possess an easily identifiable molecular structure.

2. The *boiling point temperature* is the next important entry. Boiling point is the temperature $T_b$ (in deg C) at which the vapor pressure of a liquid is equal to the atmospheric pressure on the liquid (typically, the ambient pressure). The normal boiling point is one of the few parameters known for almost every compound, which means that its value can usually be found in the right reference book, or it can be easily measured in the laboratory. Consequently, NONWATER permits the entry of the value if it is known, or approximates the value if it is not (given the molecular structure of the material). For this calculation the equation developed by Meissner (1949) is applied

$$T_b = \frac{637 \, [R_D]^{1.47} + S}{[P]} \tag{12}$$

where the parameters $[R_D]$ and $[P]$ are estimated from additive techniques for each molecular component. The constant S in Eq 12 is generally a weak function of the various chemical classes, and in our application has been set equal to a value of 14,400 to enable Eq 12 to recover the proper boiling point temperature for water.

Once these input values are known, the program can estimate all of the necessary properties from the molecular structure of the spray material.

3. The *diffusivity* is estimated from the correlation developed by Fuller, Schettler and Giddings (1966)

$$D_v = \frac{0.001 \, T_A^{1.75} \, M_r^{1/2}}{P_A \, (V_A^{1/3} + V_v^{1/3})^2} \tag{13}$$

where

$\quad V_A \quad = \quad$ molar volume of air (20.1 cu cm per mole)

$\quad V_v \quad = \quad$ molar volume of vapor (cu cm per mole)

and

$$M_r = (M_A + M_v)/M_A M_v \tag{14}$$

is the reduced molecular weight, combining the molecular weight of air $M_A$ and the molecular weight of the vapor $M_v$ (both in gm per mole).

4. The *latent heat of vaporization* is estimated from the simple method of Fishtine (1963), who modified previous work by Kistiakovskii (1921) to obtain

$$L = T_b \, (8.75 + 1.987 \ln T_b) / M_v \tag{15}$$

5. The *molal concentration* is obtained by evaluating the equation of state for the ambient temperature and pressure values.

6. The *thermal conductivity* is approximated by extending the method of Sato and Riedel (in Lyman, Reehl and Rosenblatt 1990) to vapor to obtain

$$k = \frac{0.000219}{M_v{}^{1/2}} \left[ \frac{3 + 20 \, (1 - T_A / T_c)^{2/3}}{3 + 20 \, (1 - T_b / T_c)^{2/3}} \right] \tag{16}$$

where the critical temperature is obtained from the first term in the expansion suggested by Lydersen (in Lyman, Reehl and Rosenblatt 1990)

$$T_c = T_b / 0.567 \tag{17}$$

7. The *vapor pressure coefficients B* and *C* are obtained from the expression (in Lyman, Reehl and Rosenblatt 1990)

$$\ln p_{vb} = \frac{L \, M_v \, (T_b - A)^2}{1.927 \, T_b{}^2} \left[ \frac{1}{(T_b - A)} - \frac{1}{T} \right] \tag{18}$$

where A has been set equal to zero in the second term of the Antoine equation (Eq 8 above) to be consistent with the inputs for FSCBG. This equation then gives the expressions

$$B = \frac{L \, M_v \, (T_b - A)}{1.927 \, T_b{}^2} \tag{19}$$

$$C = \frac{L \, M_v (T_b - A)^2}{1.927 \, T_b{}^2} \tag{20}$$

Overall, the most this approach can accomplish is to estimate the nonwater physical properties of the spray material, based on the simplifying approximations discussed above. In most cases these estimates will have an accuracy of ten to 35 percent, depending on the property in question. For the noncritical FSCBG input parameters (from Table 1), this level of error will not impact the final accuracy of the FSCBG predictions themselves. For the critical input parameters, the user is cautioned to run the model for a range of property values, to estimate the importance of the property in question and the final accuracy of the FSCBG predictions.

Now, we need to return to some basic evaporation modeling to see whether alternate data approaches are also possible.

Table 2: Main Menu of the NONWATER Program

```
+====================================================+
| ESTIMATION OF PROPERTIES OF ORGANIC COMPOUNDS |
|                  Main Menu                         |
+====================================================+

  1) Name of Compound
  2) Ambient Temperature              20.00      deg C
  3) Ambient Pressure                 1013.      mb
  4) Molecular Weight              needs input
  5) Boiling Point Temperature     needs input

     Diffusivity                   to be calculated
     Latent Heat of Vaporization   to be calculated
     Molal Concentration              .4229E-04 mole/cm3
     Thermal Conductivity          to be calculated
     Vapor Pressure Coefficient B  to be calculated
     Vapor Pressure Coefficient C  to be calculated

  0) EXIT

Enter choice >
```

# 5. CLASSICAL EVAPORATION

FSCBG includes an algorithm (Eq 1 and subsidiary equations detailed in Teske et al. 1993) for evaporating released material in an aerial application simulation. This model is based on the classical Fuchs approach, depending strongly upon additional equations used to represent viscosity, diffusivity, thermal conductivity, and, most especially, Sherwood number. The recovery of the required physical properties, and the extension of the Fuchs analysis to nonwater evaporation, is potentially nontrivial.

Nonetheless, significant progress has been made to date by assuming that regardless of the tank mix solution, as long as the solvent is water, the sprayed material will behave just like water when it evaporates. This approach has been used by the USDA Forest Service (and the authors of this report) in all field simulations and comparisons with deposition data to this point in time. It is a convenient approach, but one that begs the question of physical properties of the spray material. Thus, it would seem sensible to return to the most fundamental approach suggested in the literature, and see where that may lead us.

Traditional approaches to evaporation of nonwater materials tend to invoke the $D^2$-law (Lefebvre 1989), written as

$$D_0^2 - D^2 = \lambda t \tag{21}$$

where

$$
\begin{aligned}
D_0 \quad &= \quad \text{initial droplet diameter } (\mu m) \\[1em]
D \quad &= \quad \text{droplet diameter } (\mu m) \text{ at time t (sec)} \\[1em]
\lambda \quad &= \quad \text{evaporation rate (sq } \mu m \text{ per sec); a constant}
\end{aligned}
$$

This model is popular because it contains the basic physics of the evaporation process: namely, that evaporation is a surface effect and thus intimately connected with the surface area of a drop represented by the square of its diameter. And, of course, evaporation tends to follow this behavior quite well in many fields of study. Experiments have shown that Eq 21 is acceptable for small pure component drops, but may be inadequate for multi-component mixtures, or for liquid phase surface resistance (Dennison and Wedding 1984; Seaver et al. 1992).

To generalize the model for our use here requires some normalization. Two effects are included:

1. Division of Eq 21 by $D_0^2$, effectively removing dependence of the evaporation rate on the initial diameter, and collapsing all drops onto one curve.

2. Inclusion of the wet bulb temperature depression effect for water, effectively parameterizing the dependence of the evaporation rate on the temperature and relative humidity recovered for each trial experiment for each test substance. Wet bulb temperature

depression combines the dry bulb temperature and relative humidity measurements into one variable $\Delta T_{wb}$ through the Carrier equation (Jennings and Lewis 1950). Its effect has been used successfully before in the development of a simple water-based evaporation model (Trayford and Welch 1977). Using it here is a convenience that collapses data remarkably well, probably because most test substances use water as a solvent.

These two assumptions permit us to rewrite Eq 21 as

$$1 - \frac{D^2}{D_o^2} = \lambda^* \left[ \frac{t \, \Delta T_{wb}}{D_o^2} \right] \tag{22}$$

where

$$\lambda^* = \lambda / \Delta T_{wb} \text{ (sq } \mu\text{m per sec per deg C)}$$

where the evaporation rate now includes the effect of the wet bulb temperature depression. To evaluate Eq 22, we look to the available data to evaluate $\lambda^*$ as a constant for each test substance.

# 6. COLORADO STATE UNIVERSITY DATA

Dennison and Wedding (1984) conducted a wind tunnel study of evaporation rates of thirteen pesticide mixtures plus water. To our knowledge this was the first study of its kind. The spray materials are summarized in Table 3. Although these materials are somewhat dated, the available database provides a means of testing the traditional $D^2$-law as described above. To do this, we re-examine the curve fit relationships developed previously for this data (Teske 1989).

For this we must manipulate Eq 6, with the substitution $a = D_0$, squaring the expression and retaining only the lowest order terms, to arrive at

$$1 - \frac{D^2}{D_0^2} = - \frac{2\, b\, D_0}{\Delta T_{wb}} \left[ \frac{t\, \Delta T_{wb}}{D_0^2} \right] \tag{23}$$

where the evaporation rate may be taken as

$$\lambda^* = -2\, b\, D_0\, /\, \Delta T_{wb} \tag{24}$$

from a comparison with Eq 22. Thus, the previous results (Teske 1989) may be used to develop the evaporation rates summarized in Table 4. These evaporation rates are constant over the whole evaporation history of the droplet, as reported by Dennison and Wedding (1984).

Several conclusions may be drawn from this study:

1. Test substances 1, 3 and 4 are oil-based, and do not therefore evaporate. This analysis is confirmation for not invoking the evaporation model when oil is the solvent in the tank mix.

2. Water solvent behaves similar to water (although with a higher evaporation rate compared to test substance 12); changing the amount of a material added to water doesn't seem to change its evaporation rate (comparing test substances 6 and 7, and 10 and 11). This finding may imply that recovering an evaporation rate for one tank mix is all that is needed for tank mixes with different ratios of components.

3. The relative standard deviation values (standard deviation divided by the mean value) for the water-based tank mixes all seem to be at reasonable levels. A published sensitivity analysis (Teske and Barry 1993) indicates that evaporation rate in the model is a fairly insensitive parameter. These results may imply that using a single value for evaporation rate may be appropriate. In fact, the average result for all of the water-based pesticides is remarkably consistent with a single evaporation rate, although the evaporation rate is higher than that of water. Still, these findings may suggest that FSCBG be extended to include the evaporation rate equation (Eq 21) as an alternate nonwater-based evaporation algorithm.

## Table 3: Solutions Tested by Dennison and Wedding (1984)

| Substance Number | Tank Mixture |
|---|---|
| 1 | 0.5 gal Sevin-4 oil<br>0.48 gal No. 2 fuel oil<br>0.02 gal Automate Red B dye |
| 2 | 0.5 oz Polyhedra Douglas-fir Tussock Moth<br>    Nucleopolyhedrosis Virus<br>0.25 gal molasses<br>0.7 gal water<br>NaOH to bring the pH to between 6.0 and 7.2 |
| 3 | 0.8 gal Sevin-4 oil<br>0.48 gal No. 2 fuel oil<br>0.02 gal Automate Red B dye |
| 4 | 0.98 gal No. 2 fuel oil<br>0.02 gal Automate Red B dye |
| 5 | 0.5 gal Thuricide 16B<br>0.5 gal water |
| 6 | 0.5 lb Orthene 75S<br>1.0 gal water |
| 7 | 1.0 lb Orthene 75S<br>1.0 gal water |
| 8 | 2.0 qt Dow Esteron (2,4,5,-T)<br>10.0 gal water |
| 9 | 2.0 qt Dow Esteron 99<br>10.0 gal water |
| 10 | 0.5 lb Dipel<br>0.5 lb Shade<br>1.0 gal water<br>0.016692 lb Rhodamine B extra |
| 11 | 0.5 lb Dipel<br>1.0 gal water<br>0.016692 lb Rhodamine B extra |
| 12 | water |
| 13 | 5.0 oz Nalco-Trol<br>100.0 gal water |
| 14 | 10.0 oz Nalco-Trol<br>100.0 gal water |

Table 4: Evaporation Rates from the Dennison and Wedding (1984) data

| Substance Number | Evaporation Rate ($\mu m^2$/sec/deg C) | Relative Standard Deviation |
|---|---|---|
| 1 | 2.94 | 0.27 |
| 2 | 201.00 | 0.20 |
| 3 | 2.78 | 0.38 |
| 4 | 2.97 | 0.38 |
| 5 | 146.38 | 0.17 |
| 6 | 190.54 | 0.11 |
| 7 | 189.98 | 0.15 |
| 8 | 157.13 | 0.17 |
| 9 | 198.30 | 0.15 |
| 10 | 208.33 | 0.15 |
| 11 | 203.08 | 0.16 |
| 12 | 122.01 | 0.12 |
| 13 | 88.35 | 0.16 |
| 14 | 116.90 | 0.18 |
| average of 5 to 14 | 166.76 | 0.05 |

# 7. SOUTHERN RESEARCH INSTITUTE DATA

Gay and Segers (1994) recently completed a study of evaporation rates for three test substances of interest to the USDA Forest Service: WHO water, a 25 percent mixture of Sulfur 6L with water, and a 50 percent mixture of Thuricide 48LV with water. These results -- which required the development of a droplet evaporation apparatus -- were reported for all test runs as an average drop size (in μm) and overall evaporation rate (in ng per sec) for many combinations of ambient temperature, relative humidity, air velocity and drop size. A preliminary examination of the test results was made by Thistle, Teske and Barry (1993).

The difficulty with the data is that it is reported inadequately. Evaporation is a surface effect, best correlated with a change in the area of the drop as a function of time, not a change in mass of the drop as a function of time, as reported by Gay and Segers (1994). If we write an expression for the mass of the drop

$$\text{Mass} = \frac{\pi}{6} \rho_v D^3 = \frac{\pi}{6} \rho_v x^{3/2} \tag{25}$$

where $x = D^2$ for convenience, then the time derivative of Eq 25 becomes

$$\frac{d\text{Mass}}{dt} = \frac{\pi}{4} \rho_v D \frac{dD^2}{dt} \tag{26}$$

where we see that $dD^2/dt = -\lambda$ from differentiation of Eq 21. In this analysis $\lambda$ is considered a constant for a specific material; thus Eq 26 may be integrated over the time T of each droplet evaporation test to give

$$\int_0^T \frac{d\text{Mass}}{dt} \, dt = -\frac{\pi}{4} \rho_v \lambda \int_0^T D \, dt \tag{27}$$

By defining

$$\frac{dM}{dt}_{\text{ave}} = \frac{1}{T} \int_0^T \frac{d\text{Mass}}{dt} \, dt \tag{28}$$

$$D_{\text{ave}} = \frac{1}{T} \int_0^T D \, dt \tag{29}$$

we obtain

$$\frac{dM}{dt}\bigg|_{ave} = -\frac{\pi}{4} \rho_v \lambda D_{ave} \tag{30}$$

and

$$\lambda^* = \frac{4}{\pi \rho_v D_{ave} \Delta T_{wb}} \frac{dM}{dt}\bigg|_{ave} \tag{31}$$

consistent with the expansion following Eq 22. It is unclear whether the "overall evaporation rate" and "average drop size" reported in Table D-1 of Gay and Segers (1994) are in fact the expressions suggested in Eqs 28 and 29. However, we have no other information available, and must make the assumption that we can make these substitutions (otherwise the data would be difficult to interpret). Thus, we can examine all of the available data to recover the evaporation rates:

| Substance | Evaporation Rate ($\mu m^2$/sec/deg C) | Relative Standard Deviation |
|---|---|---|
| WHO water | 143.87 | 0.67 |
| Sulfur 6L (1:3) | 165.94 | 0.88 |
| Thuricide 48LV (1:1) | 112.18 | 0.73 |
| averages | 141.75 | 0.75 |

The conclusions that may be drawn from this study include:

1. WHO water in this test should be similar to "water" in the Colorado State University test. A comparison of evaporation rates gives a variance of 18.0 percent between the two tests.

2. The only comparable Thuricide product from the Colorado State University test is test substance 5, an evaporation rate variance of 23.4 percent between the two tests.

3. The average values between the two tests are nonetheless comparable (with a variance of 15.0 percent).

4. The SRI tests show a great deal of scatter, which may negate their usefulness if we restrict ourselves to very simple deterministic models, but may also indicate that nonwater evaporation is indeed a complex phenomenon, sensitive to small changes in properties and conditions we are not considering.

5. Because only evaporation rates were reported, the recovery of nonvolatile fractions was not possible (nor was it possible with the Colorado State University tests).

# 8. LPCAT DATA

Recently Hall, Kirchner and Downer (1994) of the Laboratory for Pest Control Application Technology (LPCAT) published evaporation data on various agricultural spray adjuvants. Their experimental setup consists essentially of a fish tank, where they used a microliter syringe to dispense a droplet of known size within a sealed evaporation chamber lowered into a uniform temperature water bath, permitted it to evaporate for a given period of time, then withdrew the chamber containing the drop, and calculated the volume lost. While their paper includes evaporation data on 28 tank mixes, their "evaporation rate" is reported as either $dD/dt$ or $dD^3/dt$, rather than the preferred $D^2$-law suggested in Eq 21. The following observations may be made from their work:

1. They test only big drops, and apparently cannot permit their drops to evaporate to small drops (otherwise they would be unable to recover the mass loss accurately). This restriction means that their apparatus and approach cannot be used to recover the nonvolatile fraction of the tank mix.

2. They have missed, as did Southern Research Institute, the importance of the $D^2$-law, and have chosen to publish data that is not as easily applicable as it could be. Some attempts at correcting their data only illustrate that the authors do not provide enough information in their paper to correlate their results appropriately.

3. The greatest drawback of the experiment, unfortunately, is that there is no airflow across the drop (their experiments were all for "static evaporation"). This implies that the typical evaporation processes present when drops are sprayed in an aerial application are not duplicated; their laboratory evaporation rates are therefore not necessarily consistent with the physical problem they are attempting to simulate. When a drop evaporates at rest, a vapor layer forms around the drop; this layer may effectively inhibit or impede further evaporation. With an ambient wind this vapor layer is constantly removed, and droplet evaporation proceeds as expected in all typical textbooks on the subject. Thus, the results obtained at LPCAT have limited applicability.

To illustrate, we examine their analysis of water data for five different drop sizes. For each of these drop sizes the authors found the quadratic curve fit satisfying Eq 6. Once we compute the proper evaporation rate, corrected for wet bulb temperature depression (Eq 22), we obtain an average $\lambda^*$ of 178.0 $\mu m^2$/sec/deg C, with a relative standard deviation of 0.032 (indicating a precise average value for five data points). This evaporation rate may be compared with the water results from Colorado State University of 122.01 $\mu m^2$/sec/deg C and from the SRI studies of 143.87 $\mu m^2$/sec/deg C. These latter values were developed with ambient flow over the drop, which, by Eqs 1 and 9, should produce a LARGER evaporation rate than static evaporation. Since the LPCAT data shows otherwise, the Hall, Kirchner and Downer (1994) results are suspect.

# 9. NONVOLATILE FRACTION

Besides attempting to recover the evaporation rate of nonwater spray materials, it is perhaps equally important to recover the nonvolatile fraction remaining after the evaporation process ceases. This number indicates the fraction of material (a mass or volume fraction) that will ultimately remain, and therefore be deposited. Up to this point we have always computed the fraction of solid materials added to a tank mix, and extracted the nonvolatile fraction as that answer.

But with specific nonwater materials, such as *Bacillus thuringiensis* (Bt), where the solid fraction may be difficult to interpret, recovering the nonvolatile fraction (or for that matter the evaporation rate) can be challenging. In previous work we have assumed the following nonvolatile fractions for undiluted Bt (MacNichol and Teske 1993a, 1993b and 1994):

| Substance | Nonvolatile Fraction |
|-----------|---------------------|
| Dipel 6AF | 0.50 |
| Dipel 6L | 0.90 |
| Dipel 8AF | 0.85 |
| Dipel 8L | 0.90 |
| Foray 48B | 0.85 |
| Gypchek | 0.205 |
| SAN 415 | 0.85 |
| Thuricide 32LV | 0.50 |
| Thuricide 48LV | 0.50 |
| TM BioControl-1 | 0.303 |

Recently, some effort has gone into recovering nonvolatile fractions with droplet capture on fine wire in a controlled environment (Luo et al. 1994). These experiments demonstrate that Bt evaporates much like water, and reaches the following nonvolatile fractions:

| Substance | Nonvolatile Fraction |
|-----------|---------------------|
| Dipel 6AF | 0.701 |
| Dipel 8AF | 0.423 |
| Foray 48B | 0.449 |
| Foray 76B | 0.454 |
| Thuricide 48LV | 0.446 |
| Thuricide 64LV | 0.252 |

which show clear inconsistency with previously assumed values. Additional research confirming the nonvolatile fractions would seem to be needed.

# 10. CONCLUSIONS AND RECOMMENDATIONS

The following conclusions are reached, and recommendations made:

1. Nonwater evaporation rate in FSCBG appears to be extremely sensitive to the values of the vapor pressure coefficients B and C. Consequently, these coefficients must be known accurately before using the model.

2. Nonwater evaporation rate in FSCBG appears to be insensitive to the range of values of latent heat of vaporization, molal concentration and thermal conductivity examined here. Consequently, it is suggested that these model inputs may be taken at their water-based values, even with nonwater evaporation.

3. A property estimation program NONWATER has been developed to approximate the remaining nonwater physical parameters needed in the FSCBG nonwater evaporation algorithm.

4. Classical evaporation rates support the $D^2$-law, verified by a series of laboratory experiments.

5. Multi-component evaporation conditions require painstaking evaluation of constants in the equations, again pointing to the alternate approach of deducing evaporation characteristics based on experiment.

Additional work in this area should be directed toward recovering evaporation rates and nonvolatile fractions of tank mixes that are not mostly water, and implementing the $D^2$ power law into FSCBG. Detailed droplet evaporation data could also be obtained through the use of far more sophisticated measuring devices (such as an electrodynamic balance, wherein charged particles are held in place within a controlled test chamber). Maintaining the water-based approximation in nonwater spray applications appears reasonable, so long as the correct nonvolatile fraction is used.

# 11. ACKNOWLEDGMENTS

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# APPENDIX: NONWATER USER MANUAL

This appendix explains the operation of the computer program NONWATER, used to estimate properties of evaporating materials. NONWATER is an interactive computer program in which all inputs are keyed into the program as prompted, while the computed results are output to the screen (an ASCII file, named NONWATER.PRT, is always maintained with the latest contents of the screens, should the user wish to print the file after leaving the program).

To begin the program, the user types NONWATER at the prompt. The summary screen then appears:

```
+====================================================+
| ESTIMATION OF PROPERTIES OF ORGANIC COMPOUNDS |
|                   Main Menu                        |
+====================================================+

1) Name of Compound
2) Ambient Temperature            20.00      deg C
3) Ambient Pressure               1013.      mb
4) Molecular Weight          needs input
5) Boiling Point Temperature needs input

   Diffusivity                    to be calculated
   Latent Heat of Vaporization    to be calculated
   Molal Concentration                .4229E-04 mole/cm3
   Thermal Conductivity           to be calculated
   Vapor Pressure Coefficient B   to be calculated
   Vapor Pressure Coefficient C   to be calculated

0) EXIT

Enter choice >
```

The user moves through the program by entering one of the numbers in the left column and pressing the ENTER key. An entry of "0" exits the program. Once items 2 through 5 have been entered, NONWATER will compute the six parameters currently shown as "to be calculated."

The first entry line permits the user to enter the name of the specific compound about to be developed (for information only). An entry of "1" leads to the submenu:

```
Enter compound name >
```

where the provided name (and ENTER) will place the name at item 1 in the Main Menu.

The second and third lines provide entries for the ambient temperature and pressure. The default values shown are those assumed whenever the user first enters the program. An entry of "2" or "3" lead to the submenus:

```
Enter temperature in deg C (20.0) >
```

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```
Enter pressure in mb (1013.) >
```

where the present values are shown in the parenthesis.

The first property of the compound to be developed is its *molecular weight* (in grams per mole). An entry of "4" at the Main Menu leads to the submenu:

```
+================================+
| MOLECULAR WEIGHT OF COMPOUND |
+================================+

Enter the chemical components of the compound element by element:
* An entry of "list" lists the inputs so far
* An entry of "new" or "clear" clears the input list
* An entry of "help" or "?" lists the possible elements
* An entry of a blank line terminates input

Element (  0 in list) >
```

This submenu works the same way as the Main Menu, by (in this case) entering the atomic symbol for one of the elements in the spray material, which then leads to the additional menu:

```
Number of occurrences in the compound >
```

With an entry of "help" at the "Element" submenu, all of the possible elements in the periodic table are listed on the screen. If we were to enter water as the spray material, we would enter the four responses "h", "2", "o", and "1", which would show with a "list" command:

```
H      2
O      1
```

Entering a blank line and ENTER returns the user to the Main Menu with a Molecular Weight of 18.02 g/mol, the correct value.

The second property of the compound to be developed is its boiling point temperature (in deg C). An entry of "5" at the Main Menu leads to the submenu:

```
+==============================+
| BOILING POINT TEMPERATURE |
+==============================+

Current boiling point temperature is computed

 1) Enter boiling point temperature (if known)
 2) Compute boiling point temperature

Enter choice >
```

With an entry of "1", the program will ask:

```
Enter boiling point temperature in deg C >
```

and return to the Main Menu, while with an entry of "2" the program will approximate the temperature before returning to the Main Menu.

When the user returns to the Main Menu now, all evaporation parameters will be estimated by the techniques described in the report. Changing ambient temperature and pressure will adjust these parameters accordingly.

NONWATER maintains its present input value status in an ASCII file called NONWATER.DAT, and a copy of the screen results in an ASCII file called NONWATER.PRT, which may be printed to provide hard copy of the results.